

Thomas Wellens^{1,2}, Marek Kuś¹¹Center for Theoretical Physics, Polish Academy of Sciences, al. Lotników 32/46, PL-02-668 Warszawa, Poland,²MPI für Physik komplexer Systeme, Nöthnitzer Str. 38, D-01187 Dresden, Germany

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We describe a purely algebraic method for finding the best separable approximation [1] to a mixed state of a composite 2×2 quantum system, consisting of a decomposition of the state into a linear combination of a mixed separable part and a pure entangled one. We prove that, in a generic case, the weight of the pure part in the decomposition equals the concurrence of the state.

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I. INTRODUCTION

One of the main interests of quantum information theory concerns the nonclassical features connected with the nonseparability (or entanglement) of states of composite systems. Since entanglement plays a crucial role in various applications in quantum information processing, the problem of characterization of entangled states is of a paramount importance.

It is easy to check whether a *pure* state of a composite system is separable or entangled. The situation complicates in the case of mixed states. A simple and practical necessary criterium of separability is known, but there are no known sufficient conditions for higher dimensional composite systems.

Recently [1], a very interesting description of entanglement was achieved by defining the best separable approximation (BSA) of a mixed entangled state. In the simplest case of a 2×2 dimensional composite system, it consists of a decomposition of the state into a linear combination of a mixed separable part and a pure entangled one. In this way, the whole nonseparability properties are concentrated in the pure part. It also provides a natural measure of entanglement given by the entanglement of the pure part (well defined for the pure states) multiplied by the weight of the pure part in the decomposition.

In the original paper [1], the authors proposed a numerical method for finding the BSA in 2×2 systems. Some analytical results for special states were found in [2]. In this paper, we show how to find the BSA of an arbitrary 2×2 state ρ in a purely algebraic way, without employing any maximization or optimization procedure. As a byproduct, we prove that, in the case that the BSA ρ_s of ρ is of rank 4, the weight with which the entangled part enters the decomposition leading to the BSA, equals another measure of entanglement, namely the concurrence of ρ [3]. Furthermore, the pure part is maximally entangled in this case (the last fact was recently proved by other means in [4]).

The situation is more complicated if the BSA ρ_s is not of full rank. As we will show, for $\text{rank}(\rho) = 4$ but $\text{rank}(\rho_s) < 4$ the components of the BSA are determined by a set of two nonlinear equations which can be easily solved numerically, whereas the case of a degenerate ρ (i.e. $\text{rank}(\rho) < 4$) can be treated as a limiting case of the full-rank one. It is to stress that in these cases there is no simple relation between the concurrence of the state and the weight of the entangled part as we were able to prove for $\text{rank}(\rho_s) = 4$. Presently, we do not have a simple explanation or interpretation of this fact which deserves further investigations.

The paper is organized as follows. In Section II we give a maximally shortened account on separability and entanglement of mixed states. The main results of the paper are formulated and proved in Section III. The technical lemmas used in the proofs of the two main theorems of Section III are relegated to two Appendices - the first contains some more general theorems concerning properties of mixed states of 2×2 systems, whereas the second one is mainly devoted to a technical lemma concerning relations between spectra of two important matrices obtained from the initial mixed state.

II. SEPARABILITY AND ENTANGLEMENT OF MIXED STATES

A mixed state ρ of a bipartite quantum system is separable if it is a convex combination of product states [5]

$$\rho = \sum_i^k p_i \rho_i^A \otimes \rho_i^B, \quad p_i \geq 0, \quad \sum_i^k p_i = 1, \quad (2.1)$$

where ρ_i^A, ρ_i^B are legitimate (i.e. hermitian and positive definite) density matrices of the subsystems. As observed in [6], a necessary condition for separability of ρ is that its *partial transposition*, defined as

$$\rho^{T_B} := \sum_i^k p_i \rho_i^A \otimes (\rho_i^B)^T, \quad (2.2)$$

is positive definite, i.e. is also a legitimate density matrix for the composite system. (Here, we define the operation of partial transposition by Eq (2.2) also in the case of an arbitrary, not necessarily separable state, when ρ_i^A and ρ_i^B do not need to be positive or/and p_i are not all positive - such a decomposition obviously exists for an arbitrary ρ). For low dimensional (2×2 and 2×3) systems the above condition is also sufficient [7].

Obviously, the result of partial transposition depends on the basis in subspace \mathcal{H}_B . If we change the bases of \mathcal{H}_A and \mathcal{H}_B by a local transformation $U \otimes V$, i.e. by unitary rotations U and V in the spaces \mathcal{H}_A and \mathcal{H}_B respectively (in fact, since the overall phase factor does not play any role, we can assume $\det U = 1 = \det V$, i.e. $U, V \in SU(2)$), the matrix ρ will be transformed according to

$$\rho' = U \otimes V \rho (U \otimes V)^\dagger = \sum_i^k p_i U \rho_i^A U^\dagger \otimes V \rho_i^B V^\dagger. \quad (2.3)$$

Consequently, the partial transposition gives

$$\rho'^{T_B} = \sum_i^k p_i U \rho_i^A U^\dagger \otimes (V \rho_i^B V^\dagger)^T = U \otimes V^* \rho^{T_B} (U \otimes V^*)^\dagger, \quad (2.4)$$

where asterisk denotes the complex conjugation. From (2.4) it follows that the spectrum of ρ^{T_B} is basis-independent.

Observe also the following form of the definition of partial transpose

$$\langle e, f | \rho | e, f \rangle = \langle e, f^* | \rho^{T_B} | e, f^* \rangle, \quad (2.5)$$

where $|e, f\rangle$ denotes the product vector $|e\rangle \otimes |f\rangle$.

In order to quantify the degree of entanglement of two qubit systems, the *concurrence* was introduced in [3], defined as

$$c(\rho) = \max\{0, c_1 - c_2 - c_3 - c_4\}, \quad (2.6)$$

where $c_1 \geq c_2 \geq c_3 \geq c_4$ are the square roots of the (real and positive) eigenvalues of the matrix

$$X := \Sigma \rho^* \Sigma \rho, \quad \Sigma = \sigma_2 \otimes \sigma_2, \quad \sigma_2 := \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \quad (2.7)$$

It is a matter of a straightforward calculation to prove that the concurrence of a pure state,

$$|\psi\rangle = a_1|00\rangle + a_2|01\rangle + a_3|10\rangle + a_4|11\rangle = [a_1, a_2, a_3, a_4]^T,$$

equals

$$c(\psi) = 2|a_1 a_4 - a_2 a_3| = |\langle \psi | \Sigma | \psi^* \rangle|. \quad (2.8)$$

Due to the normalization condition $1 = \langle \psi | \psi \rangle = |a_1|^2 + |a_2|^2 + |a_3|^2 + |a_4|^2$, we have $0 \leq c(\psi) \leq 1$. The maximum $c(\psi) = 1$ is attained for the states called maximally entangled. The degree of entanglement (i.e. the concurrence) is invariant with respect to local unitary transformations (i.e. transformations of the form $U \otimes V$).

By local transformation, a pure state can be brought to its Schmidt form $|\psi\rangle = \lambda_1 e_1 \otimes f_1 + \lambda_2 e_2 \otimes f_2$, where $\{e_1, e_2\}$ and $\{f_1, f_2\}$ are appropriately chosen bases in \mathcal{H}_A and \mathcal{H}_B . In these bases thus $\psi = [\lambda_1, 0, 0, \lambda_2]^T$ and it is easy to show that the most general form of a maximally entangled state in the original bases reads

$$|\psi\rangle = a_1|00\rangle + a_2|01\rangle \mp (a_2^*|10\rangle - a_1^*|11\rangle) = \begin{bmatrix} a_1 \\ a_2 \\ \mp a_2^* \\ \pm a_1^* \end{bmatrix}, \quad |a_1|^2 + |a_2|^2 = \frac{1}{2}. \quad (2.9)$$

Let ρ be a generic density matrix for a two qubit system, i.e. a strictly positive definite (i.e. rank 4) 4×4 hermitian matrix of unit trace. According to [1], ρ has a unique decomposition of the form:

$$\rho = (1 - \lambda) |\psi\rangle \langle \psi| + \lambda \rho_s, \quad (3.1)$$

where ρ_s is a separable density matrix, $|\psi\rangle$ is a pure entangled state, and the parameter $\lambda \in [0, 1]$ is maximal. In the following, we will refer to Eq. (3.1) as the *optimal decomposition* of ρ . The separable part ρ_s is called the *best separable approximation* (BSA) of ρ , and λ its *separability*. In this section, we will prove the following

Theorem 1. Let ρ be an entangled state with $\text{rank}(\rho) = 4$. $\rho = (1 - \lambda) |\psi\rangle \langle \psi| + \lambda \rho_s$ is the optimal decomposition of ρ if and only if:

$\text{rank}(\rho_s^{T_B}) = 3$, i.e. $\exists_{|\phi\rangle} \rho_s^{T_B} |\phi\rangle = 0$, and either

(i) $\exists_{\alpha > 0} [|\phi\rangle \langle \phi|]^{T_B} |\psi\rangle = -\alpha |\psi\rangle$, or

(ii) $\text{rank}(\rho_s) = 3$, i.e. $\exists_{|\tilde{\phi}\rangle} \rho_s |\tilde{\phi}\rangle = 0$, and $\exists_{\alpha, \nu \geq 0} \left[\nu |\tilde{\phi}\rangle \langle \tilde{\phi}| + [|\phi\rangle \langle \phi|]^{T_B} \right] |\psi\rangle = -\alpha |\psi\rangle$.

According to Lemma 2 of Appendix A, $|\psi\rangle$ is maximally entangled in case (i).

The first condition, $\text{rank}(\rho_s^{T_B}) = 3$ simply states that the BSA ρ_s lies on the boundary between the set of separable and the set of entangled states, whereas conditions (i) and (ii) describe the relation between the entangled and separable part of the optimal decomposition. Remarkably, the only relevant properties of ρ_s are the vectors $|\phi\rangle$, and possibly $|\tilde{\phi}\rangle$, in the kernels of $\rho_s^{T_B}$ and ρ_s .

Theorem 1 allows us to check immediately if a given decomposition of ρ is the optimal one. It also simplifies the construction of the BSA for a given ρ . Indeed, case (i), i.e. any BSA with rank 4, can be solved explicitly, according to the following

Theorem 2. If the BSA ρ_s of ρ has full rank, the vector $|\phi\rangle$ in the (one-dimensional, see Theorem 1) kernel of $\rho_s^{T_B}$ is an eigenvector of

$$Y = \Sigma \rho^{T_A} \Sigma \rho^{T_B} \quad (3.2)$$

belonging to the smallest eigenvalue γ of Y . The weight $1 - \lambda$ of the entangled part in the optimal decomposition is given by $1 - \lambda = 2\sqrt{\gamma} = c(\rho)$, where $c(\rho)$ is the concurrence of ρ .

Theorem 2 provides a connection between the BSA and the concurrence of ρ , which was originally [8] introduced as an auxiliary quantity in order to calculate the entanglement of formation [9]. Apart from the explicit formula (2.6), the concurrence of a mixed state is defined as the minimum of the average concurrence $\langle c \rangle = \sum_i p_i c(\psi_i)$ over all decompositions $\rho = \sum_i p_i |\psi_i\rangle \langle \psi_i|$ of ρ into pure states. After decomposing ρ_s into product states, also the BSA, Eq. (3.1), defines a particular decomposition, and it follows that

$$c(\rho) \leq (1 - \lambda) c(\psi). \quad (3.3)$$

This inequality implies $c(\rho) + \lambda \leq 1$, which has already been conjectured in [11]. According to Theorem 2, equality in Eq. (3.3) holds if the BSA of ρ has full rank (in this case, $c(\psi) = 1$). In other words: the decomposition (3.1) is also optimal in the sense that it minimizes the average concurrence. One might assume that this is true in general, i.e. also in the second case, $\text{rank}(\rho_s) = 3$. Indeed, there exist examples where the inequality (3.3) is saturated also in this case, e.g. the generalized Werner states $\rho = x |\phi\rangle \langle \phi| + \frac{1-x}{4} \mathbb{I}$, with $|\phi\rangle$ not maximally entangled. (The optimal decomposition of these states is given in [2].) In general, however, we have found that the equality in (3.3) does *not* always hold. Hence, the concurrence of ρ and the quantity $(1 - \lambda) c(\psi)$ provide two inequivalent measures of entanglement. Indeed, it is straightforward to show that $(1 - \lambda) c(\psi)$ really *is* a good measure of entanglement, i.e. it fulfills the following three conditions [10]: it vanishes if and only if ρ is separable, is invariant under local unitary operations and its expectation value is non-increasing under general local operations (see [10] for details).

Before we present the proofs of Theorem 1 and 2, we want to demonstrate how to use the above results in order to construct the BSA for a given entangled ρ of rank 4: first, we calculate the smallest eigenvalue γ and the corresponding eigenvector $|\phi\rangle$ of the 4×4 matrix Y , given by Eq. (3.2). (The eigenvalue γ is not degenerate, see Lemma 7.) Then, we obtain $|\psi\rangle$ from condition (i) of Theorem 1, $\lambda = 1 - 2\sqrt{\gamma}$, and ρ_s from Eq. (3.1). If ρ_s is positive and separable, it is the BSA according to Theorem 1. (It is not necessary to check $\rho_s^{T_B} |\phi\rangle = 0$, since this follows from the construction of $|\phi\rangle$, see Lemma 7 and Lemmas 3-5.) If not, the BSA has rank 3, and from the second case of Theorem 1 we obtain the following set of equations:

$$[\rho|\tilde{\phi}\rangle\langle\tilde{\phi}|\rho]^{T_B}|\phi\rangle = \langle\tilde{\phi}|\rho|\tilde{\phi}\rangle\rho^{T_B}|\phi\rangle, \quad (3.4)$$

$$\nu|\tilde{\phi}\rangle\langle\tilde{\phi}|\rho|\tilde{\phi}\rangle + [|\phi\rangle\langle\phi|]^{T_B}\rho|\tilde{\phi}\rangle = -\alpha\rho|\tilde{\phi}\rangle. \quad (3.5)$$

Here, we used $|\psi\rangle = \rho|\tilde{\phi}\rangle$ and $(1-\lambda)^{-1} = \langle\tilde{\phi}|\rho|\tilde{\phi}\rangle$, see Eqs. (3.21) and (3.22) below. These equations can be solved numerically for $|\tilde{\phi}\rangle$, $|\phi\rangle$, α , and ν . Possibly, there exist several solutions, but only one with $\alpha, \nu \geq 0$ and which yields a positive and separable state ρ_s via Eq. (3.1). Thereby, we have found the BSA of ρ in a purely algebraic way, without employing any maximization or optimization procedure.

Finally, we want to show how far this method can be used if $\text{rank}(\rho) < 4$, in particular if $\text{rank}(\rho) = 3$, since the case $\text{rank}(\rho) = 2$ has already been solved analytically [2]. First, we note that any density matrix ρ can be obtained as a limit from the case of full rank. Thereby, we obtain the following limiting case of Theorem 1 (the complete proof will be given below):

Corollary. Let ρ be an entangled state with $\text{rank}(\rho) < 4$. $\rho = (1-\lambda)|\psi\rangle\langle\psi| + \lambda\rho_s$ is the optimal decomposition if and only if:

$$\exists_{|\phi\rangle}\rho_s^{T_B}|\phi\rangle = 0, \quad c(\phi) > 0, \quad \exists_{|\tilde{\phi}\rangle}\rho_s|\tilde{\phi}\rangle = 0, \quad \text{and} \quad \exists_{\alpha, \nu \geq 0} \left[\nu|\tilde{\phi}\rangle\langle\tilde{\phi}| + [|\phi\rangle\langle\phi|]^{T_B} \right] |\psi\rangle = -\alpha|\psi\rangle. \quad (3.6)$$

Although Eq. (3.6) is nearly identical to case (ii) of Theorem 1, it may also arise as a limit from case (i) (with $\nu = 0$). Unlike in Theorem 1, we must explicitly demand that $c(\phi) > 0$ (in order to exclude solutions which would not correspond to the optimal decomposition, see proof of the corollary).

For the solution of Eq. (3.6), the following observation is helpful (cf. Lemma 1 of [1]): if $|\tilde{\phi}\rangle$ is not in the kernel of ρ , then $|\psi\rangle = \rho|\tilde{\phi}\rangle$ and λ is given by Eq. (3.21) (well defined, since $|\psi\rangle$ is in the range of ρ). Consequently, Eq. (3.6) reduces to Eqs. (3.4,3.5), as in the case of full rank (with the additional constraint $c(\phi) > 0$). Hence, the recipe for obtaining the BSA of ρ with $\text{rank}(\rho) = 3$ is as follows: first, try to find a solution of Eqs. (3.4,3.5) with $\alpha, \nu \geq 0$ and $c(\phi) > 0$ which yields a positive and separable ρ_s . If such a solution does not exist, we know that $|\tilde{\phi}\rangle$ must be in the kernel of ρ , which uniquely determines $|\tilde{\phi}\rangle$ (since we assumed $\text{rank}(\rho) = 3$). Then, Eq. (3.6) can be solved numerically for $|\psi\rangle$, $|\phi\rangle$, α , ν and λ (after inserting $|\tilde{\phi}\rangle$ and replacing $\rho_s^{T_B}$ by $\rho^{T_B} - (1-\lambda)[|\psi\rangle\langle\psi|]^{T_B}$). Furthermore, the following fact may be useful: if the kernel of ρ contains a product vector $|e, f\rangle$, then the solution of Eq. (3.6) fulfills $|\tilde{\phi}\rangle \perp |e, f\rangle$ and $|\phi\rangle \perp |e, f^*\rangle$ (see proof of the corollary).

A. Proof of Theorem 1

Let ρ_s , as given by Eq. (3.1), be the BSA of ρ . The maximality condition for λ and the uniqueness of the BSA [1] imply [2]:

- (a) the state $\rho_s + \epsilon|\psi\rangle\langle\psi|$ is non-separable for $\epsilon > 0$, and
- (b) the state $\rho - (1-\lambda)|\psi'\rangle\langle\psi'|$ is either non-separable or non-positive for each $\psi' \neq \psi$.

In order to compact the notation we shall use in the following the notation $\mu = 1 - \lambda$.

According to the Peres-Horodecki criterion of separability [6,7], condition (a) implies:

$$\forall_{\epsilon > 0} \exists_{|\phi_\epsilon\rangle} \langle\phi_\epsilon| \rho_s^{T_B} + \epsilon[|\psi\rangle\langle\psi|]^{T_B} |\phi_\epsilon\rangle < 0. \quad (3.7)$$

On the other hand, since ρ_s is separable, the same criterion establishes the positivity of $\rho_s^{T_B}$. Thus, from (3.7) and the continuity argument, there is such ϕ that

$$\rho_s^{T_B}|\phi\rangle = 0. \quad (3.8)$$

Since we assumed $\text{rank}(\rho) = 4$ and the rank of a projection is one, the rank of ρ_s must be at least three. Then $\text{rank}(\rho_s^{T_B}) = 3$, as a consequence of Lemma 1 (c.f. Appendix A).

Now we exploit condition (b). Let's consider

$$\lambda\rho'_s := \rho - \mu|\psi'\rangle\langle\psi'|, \quad (3.9)$$

with

$$|\psi'\rangle = \frac{|\psi\rangle + \epsilon|\Delta\psi\rangle}{\sqrt{1 + \epsilon^2}}, \quad (3.10)$$

where $\langle \Delta\psi | \Delta\psi \rangle = 1$ and $\langle \psi | \Delta\psi \rangle = 0$. (Obviously, any pure state can be written in this form.)

To the two lowest orders in ϵ we have:

$$\lambda \rho'_s = \lambda \rho_s - \mu (\epsilon |\psi\rangle \langle \Delta\psi| + \epsilon |\Delta\psi\rangle \langle \psi| + \epsilon^2 |\Delta\psi\rangle \langle \Delta\psi| - \epsilon^2 |\psi\rangle \langle \psi|). \quad (3.11)$$

In the following, we consider separately two cases of different ranks of ρ .

(i) $\text{rank}(\rho_s) = 4$

Then, for ϵ small enough, ρ'_s is positive definite for each $|\Delta\psi\rangle$. According to the optimality condition (b) above, ρ'_s must be non-separable, i.e. there exists such $|\phi'\rangle$ that $\langle \phi' | \rho'^{T_B}_s | \phi' \rangle < 0$.

Since $\rho_s^{T_B}$ has rank 3,

$$|\phi'\rangle = |\phi\rangle + |\Delta\phi\rangle, \quad (3.12)$$

with $|\Delta\phi\rangle \rightarrow 0$ if $\epsilon \rightarrow 0$. Now from (3.8) we obtain, to the first order in ϵ :

$$\langle \Delta\phi | \lambda \rho_s^{T_B} | \Delta\phi \rangle - \mu \epsilon \langle \phi | [|\psi\rangle \langle \Delta\psi| + |\Delta\psi\rangle \langle \psi|]^{T_B} | \phi \rangle \leq 0. \quad (3.13)$$

But ρ_s is, by assumption, separable; consequently $\rho_s^{T_B}$ is positive definite

$$\langle \Delta\phi | \lambda \rho_s^{T_B} | \Delta\phi \rangle \geq 0, \quad (3.14)$$

and (3.13) implies

$$\langle \phi | [|\psi\rangle \langle \Delta\psi| + |\Delta\psi\rangle \langle \psi|]^{T_B} | \phi \rangle \geq 0, \quad (3.15)$$

which can be equivalently written as

$$\text{Tr} \left\{ [|\psi\rangle \langle \Delta\psi| + |\Delta\psi\rangle \langle \psi|]^{T_B} | \phi \rangle \langle \phi| \right\} \geq 0. \quad (3.16)$$

For arbitrary operators A and B we have $\text{Tr} A^{T_B} B = \text{Tr} A B^{T_B}$, thus from (3.16) we obtain

$$\text{Tr} \left\{ [|\psi\rangle \langle \Delta\psi| + |\Delta\psi\rangle \langle \psi|] [|\phi\rangle \langle \phi|]^{T_B} \right\} \geq 0. \quad (3.17)$$

This, however, is equivalent to

$$\langle \Delta\psi | [|\phi\rangle \langle \phi|]^{T_B} | \psi \rangle + \langle \psi | [|\phi\rangle \langle \phi|]^{T_B} | \Delta\psi \rangle \geq 0 \quad (3.18)$$

for all $|\Delta\psi\rangle \perp |\psi\rangle$. Since (3.18) is linear in $|\Delta\psi\rangle$, changing $|\Delta\psi\rangle$ into $-|\Delta\psi\rangle$ reverses the inequality, hence in fact it must be that

$$\langle \Delta\psi | [|\phi\rangle \langle \phi|]^{T_B} | \psi \rangle = 0. \quad (3.19)$$

The above equality must be fulfilled by all $|\Delta\psi\rangle \perp |\psi\rangle$. This is possible only if $|\psi\rangle$ is an eigenvector of $A = [|\phi\rangle \langle \phi|]^{T_B}$. (Note that, although T_B and $|\phi\rangle$ depend on the local basis of \mathcal{H}_B , the operator A is basis-independent, i.e. transforms in the usual way, Eq. (2.3), under local unitary transformations.) To arrive at the first case (i) of Theorem 1, it remains to be shown that the sign of the corresponding eigenvalue α is negative. This, however, follows from the limit $\epsilon \rightarrow 0$ of Eq. (3.7)

$$\langle \phi | [|\psi\rangle \langle \psi|]^{T_B} | \phi \rangle \leq 0, \quad (3.20)$$

after using again the identity $\text{Tr} A^{T_B} B = \text{Tr} A B^{T_B}$. Furthermore, α cannot be zero - otherwise (according to Lemma 2) $|\phi\rangle$ would be a separable, i.e. a product state: $|\phi\rangle = |e, f\rangle$, and since $\rho_s^{T_B} |e, f\rangle = 0$ (c.f. (3.8)), we have $\rho_s |e, f^*\rangle = 0$, which contradicts the assumption $\text{rank}(\rho_s) = 4$. From Lemma 2 (c.f. Appendix) we infer that $|\psi\rangle$ is maximally entangled. This provides an alternative proof of the fact proved in [4] that if ρ and ρ_s are of maximal rank then $|\psi\rangle$ in (3.1) is maximally entangled.

(ii) Second case: $\text{rank}(\rho_s) < 4$

We assumed that ρ has rank 4, so $\text{rank}(\rho_s) = 3$. From Lemma 1 in [1], we know that

$$1 - \lambda = \frac{1}{\langle \psi | \rho^{-1} | \psi \rangle}. \quad (3.21)$$

Furthermore, it is easy to check that

$$|\tilde{\phi}\rangle = \rho^{-1}|\psi\rangle \quad (3.22)$$

fulfills $\rho_s|\tilde{\phi}\rangle = 0$. Since $\text{rank}(\rho_s) = 3$, ρ'_s , Eq.(3.11), is positive definite if

$$\langle \tilde{\phi} | (\epsilon|\psi\rangle\langle\Delta\psi| + \epsilon|\Delta\psi\rangle\langle\psi| + \epsilon^2|\Delta\psi\rangle\langle\Delta\psi| - \epsilon^2|\psi\rangle\langle\psi|) | \tilde{\phi} \rangle < 0. \quad (3.23)$$

Obviously, this condition is fulfilled if $|\Delta\psi\rangle \perp |\tilde{\phi}\rangle$. [$\langle\psi|\tilde{\phi}\rangle \neq 0$ follows from Eq. (3.21).] Hence (as in case 1), all such $|\Delta\psi\rangle$ must fulfill Eq. (3.19).

This is equivalent to

$$(1 - |\psi\rangle\langle\psi| - |\tilde{\psi}\rangle\langle\tilde{\psi}|) [|\phi\rangle\langle\phi|]^{T_B} |\psi\rangle = 0, \quad (3.24)$$

where $|\tilde{\psi}\rangle$ is defined such that $|\tilde{\psi}\rangle \perp |\psi\rangle$ and $|\tilde{\psi}\rangle$ and $|\psi\rangle$ span the same two-dimensional subspace as $|\tilde{\phi}\rangle$ and $|\psi\rangle$. (We assume that $|\psi\rangle \neq |\tilde{\phi}\rangle$; otherwise, ρ'_s is positive for all $|\Delta\psi\rangle$, and we get the same result as in the first case, which below will turn out to be a special case of the result in the second case.)

We still have to check the case $|\Delta\psi\rangle = |\tilde{\psi}\rangle$. Then, it is always possible to multiply $|\Delta\psi\rangle$ by a phase factor such that ρ'_s is positive, see Eq. (3.23) in first order of ϵ . This leads us (as in case 1) to Eq. (3.18). It follows that

$$-\nu \langle \tilde{\psi} | \tilde{\phi} \rangle \langle \tilde{\phi} | \psi \rangle = \langle \tilde{\psi} | [|\phi\rangle\langle\phi|]^{T_B} | \psi \rangle \quad (3.25)$$

with a nonnegative real parameter ν . Otherwise, $|\Delta\psi\rangle$ could be multiplied by a phase factor such that Eq. (3.23) is fulfilled and Eq. (3.18) not. (Note that $\langle\tilde{\psi}|\tilde{\phi}\rangle\langle\tilde{\phi}|\psi\rangle \neq 0$, since $\langle\psi|\tilde{\phi}\rangle \neq 0$ follows from Eq. (3.21), and $\langle\tilde{\psi}|\tilde{\phi}\rangle \neq 0$ from the construction of $\tilde{\psi}$.)

The two conditions Eqs. (3.25,3.24) are equivalent to the following condition: $|\psi\rangle$ is an eigenvector of the operator

$$A = \nu|\tilde{\phi}\rangle\langle\tilde{\phi}| + [|\phi\rangle\langle\phi|]^{T_B}. \quad (3.26)$$

To complete the first part of the proof of Theorem 1, we will show now that the corresponding eigenvalue α cannot be positive.

As a consequence of Lemma 2, A has at least three nonnegative eigenvalues. However, there is also at least one nonpositive eigenvalue. This follows from the existence of a product vector $|e, f\rangle \in R(\rho_s)$ such that $|e, f^*\rangle \in R(\rho_s^{T_B})$, as shown in [4], which implies $\langle e, f | A | e, f \rangle = 0$. Furthermore, A cannot have more than one zero eigenvalue: otherwise, $|\phi\rangle$ would have to be a product vector (see Lemma 2), and $|\tilde{\phi}\rangle$ would be the corresponding partially transposed product vector. Hence, $|\tilde{\phi}\rangle\langle\tilde{\phi}|$ and $[|\phi\rangle\langle\phi|]^{T_B}$ would be identical and proportional to A , and $|\psi\rangle$, as an *entangled* eigenvector of A , would have to be perpendicular to $|\tilde{\phi}\rangle$, i.e. $\text{rank}(\rho) = 3$, which contradicts the assumption $\text{rank}(\rho) = 4$.

The above considerations about the spectrum of A are useful for the following reason: let us assume that there exists an entangled state ρ' with $\alpha' < 0$ which has the property that $\rho(x) = x\rho + (1-x)\rho'$ is entangled for $x \in [0, 1]$. (ρ' may be a state with BSA of rank 4, for which we have already shown above that $\alpha' < 0$.) Now, the optimal decomposition (3.1) - in particular the eigenvalue $\alpha(x)$ - changes smoothly when varying x from 0 to 1 (this follows from the uniqueness of the optimal decomposition). Since, as shown above, A (having one nonpositive and three nonnegative eigenvalues) cannot have two zero eigenvalues, a crossing of eigenvalues at zero is not possible, and $\alpha = \alpha(1) \leq 0$ follows from $\alpha' = \alpha(0) < 0$.

It remains to be shown that a state ρ' with the above properties exists. For this purpose, we consider the Werner states $\rho' = y|\psi'\rangle\langle\psi'| + \frac{1-y}{4}\mathbb{I}$, with maximally entangled $|\psi'\rangle$. For these states, it has been shown in [2] that

the pure state in the optimal decomposition equals $|\psi'\rangle$ and $\lambda' = 3(1-y)/2$. It follows that $\text{rank}(\rho'_s) = 4$, and $\alpha' < 0$, as shown above (first case). Now, we choose $|\psi'\rangle$ as the eigenvector of $[[\chi]\langle\chi|]^{T_B}$ with negative eigenvalue (such an eigenvalue exists according to Lemma 2), where $|\chi\rangle$ is an entangled pure state with $\langle\chi|\rho^{T_B}|\chi\rangle < 0$ (exists, since ρ is entangled). Using $\langle\psi'|[[\chi]\langle\chi|]^{T_B}|\psi'\rangle = \langle\chi|[[\psi']\langle\psi'|]^{T_B}|\chi\rangle$, it follows that $\langle\chi|(\rho')^{T_B}|\chi\rangle < 0$ for large enough y , hence also $\langle\chi|\rho(x)^{T_B}|\chi\rangle < 0$ for $x \in [0, 1]$, i.e. $\rho(x)$ is entangled.

Finally, we will prove the reverse direction of Theorem 1, i.e. that both cases (i) and (ii) are also *sufficient* for the optimality of the decomposition (3.1). For this purpose, let us assume that there exists another decomposition with larger λ . Then, because of the convexity of the set of separable states, such a decomposition with larger λ also exists in the infinitesimal neighborhood of $\{\lambda, |\psi\rangle\}$. Hence, for each (infinitesimal small) $\epsilon > 0$, there exists $\lambda' = \lambda + \Delta\lambda$ (with $\Delta\lambda > 0$ and $\Delta\lambda \rightarrow 0$ if $\epsilon \rightarrow 0$) and $|\Delta\psi\rangle \perp |\psi\rangle$ such that

$$\lambda' \rho'_s = \lambda \rho_s + \Delta\lambda |\psi\rangle\langle\psi| - (1 - \lambda') (\epsilon |\psi\rangle\langle\Delta\psi| + \epsilon |\Delta\psi\rangle\langle\psi| + \epsilon^2 |\Delta\psi\rangle\langle\Delta\psi| - \epsilon^2 |\psi\rangle\langle\psi|) \quad (3.27)$$

is separable. Now, let us assume that there exists $|\phi\rangle$ with $\rho_s^{T_B}|\phi\rangle = 0$ and either condition (i) or (ii) from Theorem (i) is fulfilled. In the following, we will show that both (i) or (ii) lead to a contradiction, since either $\langle\phi|\rho_s'^{T_B}|\phi\rangle < 0$ or $\langle\tilde{\phi}|\rho'_s|\tilde{\phi}\rangle < 0$.

(i) implies $\langle\Delta\psi|[[\phi]\langle\phi|]^{T_B}|\psi\rangle = 0$, $\langle\psi|[[\phi]\langle\phi|]^{T_B}|\psi\rangle < 0$, and $\langle\Delta\psi|[[\phi]\langle\phi|]^{T_B}|\Delta\psi\rangle > 0$. (The third inequality follows from the spectrum of $[[\phi]\langle\phi|]^{T_B}$, see Lemma 2.) Inserting into Eq. (3.27) immediately yields $\langle\phi|\rho_s'^{T_B}|\phi\rangle < 0$.

(ii) implies $\langle\psi|[[\phi]\langle\phi|]^{T_B}|\psi\rangle = \alpha - \nu\langle\psi|\tilde{\phi}\rangle\langle\tilde{\phi}|\psi\rangle$ and $\langle\Delta\psi|[[\phi]\langle\phi|]^{T_B}|\psi\rangle = -\nu\langle\Delta\psi|\tilde{\phi}\rangle\langle\tilde{\phi}|\psi\rangle$. Inserting into Eq. (3.27) yields:

$$\langle\phi|\rho_s'^{T_B}|\phi\rangle = \Delta\lambda \alpha + (1 - \lambda')\epsilon^2(\alpha - \beta) - \nu\langle\tilde{\phi}|\rho'_s|\tilde{\phi}\rangle, \quad (3.28)$$

where $\beta = \langle\Delta\psi|A|\Delta\psi\rangle$. Since $\alpha \leq 0$ and $\alpha < \beta$ (remember that $A = \nu|\tilde{\phi}\rangle\langle\tilde{\phi}| + [[\phi]\langle\phi|]^{T_B}$ has three nonnegative eigenvalues, i.e. α is the smallest eigenvalue of A), it follows that ρ'_s is either non-positive or non-separable.

□

B. Proof of Theorem 2

Let us assume that Eq. (3.1) is the optimal decomposition of ρ , with ρ_s of rank 4. According to Theorem 1 (and Lemma 2), we know that $|\psi\rangle$ is maximally entangled, i.e. $c(\psi) = 1$. Hence, we can use Lemma 3 of Appendix A to write

$$\lambda \rho_s^{T_B} = \rho^{T_B} - \mu[|\psi\rangle\langle\psi|]^{T_B} = \rho^{T_B} - \mu\left(\frac{1}{2}\mathbb{I} - |\tilde{\psi}\rangle\langle\tilde{\psi}|\right),$$

where $|\tilde{\psi}\rangle$ is defined by

$$[|\psi\rangle\langle\psi|]^{T_B}|\tilde{\psi}\rangle = -\frac{1}{2}|\tilde{\psi}\rangle. \quad (3.29)$$

Consequently, for an arbitrary $|\phi'\rangle$

$$0 \leq \lambda\langle\phi'|\rho_s^{T_B}|\phi'\rangle = \langle\phi'|\rho^{T_B}|\phi'\rangle + \mu|\langle\phi'|\tilde{\psi}\rangle|^2 - \frac{\mu}{2}. \quad (3.30)$$

For $|\phi'\rangle = |\phi\rangle$, the above equation, due to (3.8), reads

$$0 = \langle\phi|\rho^{T_B}|\phi\rangle + \mu|\langle\phi|\tilde{\psi}\rangle|^2 - \frac{\mu}{2}. \quad (3.31)$$

Observe now that because of (i) (Theorem 1) and (3.29), we can apply Lemma 5, concluding that $|\phi\rangle$ and $|\tilde{\psi}\rangle$ have a common Schmidt basis, hence, according to Lemma 4 we can rewrite (3.31) as

$$0 = \langle\phi|\rho^{T_B}|\phi\rangle + \frac{\mu}{2}c(\phi). \quad (3.32)$$

Using the results of the same Lemma we can estimate the last two terms on the right-hand side of (3.30) by $\frac{\mu}{2}c(\phi')$:

$$0 \leq \langle \phi' | \rho^{T_B} | \phi' \rangle + \frac{\mu}{2}c(\phi'). \quad (3.33)$$

In order to simplify equations we are going to consider below, let us make the following observation. Both equation (3.32) and inequality (3.33) are bilinear in $|\phi\rangle$ if only we calculate the concurrence according to (2.8) regardless of the normalization of $|\psi\rangle$. Obviously such a quantity is not limited from above, but this will not play any role in the following. The final formula will involve only normalized vectors.

Substituting $|\phi'\rangle = |\phi\rangle + \varepsilon|\Delta\phi\rangle$ (with arbitrary ε and $|\Delta\phi\rangle$) to (3.33) and using (3.32), we obtain in the lowest order in ε

$$0 \leq \varepsilon \left(\langle \Delta\phi | \rho^{T_B} | \phi \rangle + \langle \phi | \rho^{T_B} | \Delta\phi \rangle + \frac{\mu}{2} \frac{dc(\phi + \varepsilon\Delta\phi)}{d\varepsilon} \Big|_{\varepsilon=0} \right). \quad (3.34)$$

From the definition of concurrence (2.8) we obtain

$$c(\phi + \varepsilon\Delta\phi) = c(\phi) + \varepsilon (\langle \Delta\phi | \Sigma | \phi^* \rangle + \langle \phi^* | \Sigma | \Delta\phi \rangle) + o(\varepsilon^2),$$

after adjusting the phase of $|\phi\rangle$ to make $\langle \phi | \Sigma | \phi^* \rangle$ real and positive and using $\langle \Delta\phi | \Sigma | \phi^* \rangle = \langle \phi | \Sigma | \Delta\phi^* \rangle = \langle \Delta\phi^* | \Sigma | \phi \rangle^* = \langle \phi^* | \Sigma | \Delta\phi \rangle^*$ which is a consequence of $\Sigma = \Sigma^\dagger = \Sigma^*$. Thus, we can rewrite (3.34) as

$$\langle \Delta\phi | \rho^{T_B} | \phi \rangle + \langle \phi | \rho^{T_B} | \Delta\phi \rangle + \frac{\mu}{2} (\langle \Delta\phi | \Sigma | \phi^* \rangle + \langle \phi^* | \Sigma | \Delta\phi \rangle) \geq 0, \quad (3.35)$$

valid for an arbitrary $|\Delta\phi\rangle$. Again, considering (3.35) for $|\Delta\phi\rangle$ and $-|\Delta\phi\rangle$, we conclude that in fact (3.35) is an equality

$$\langle \Delta\phi | \Psi \rangle + \langle \Psi | \Delta\phi \rangle = 0,$$

where

$$|\Psi\rangle = \rho^{T_B} |\phi\rangle + \frac{\mu}{2} \Sigma |\phi^*\rangle.$$

Since $|\Delta\phi\rangle$ is arbitrary, we have $|\Psi\rangle = 0$ and, consequently

$$\rho^{T_B} |\phi\rangle = -\frac{\mu}{2} \Sigma |\phi^*\rangle. \quad (3.36)$$

Short manipulations using $\Sigma^2 = 1$ allow for rewriting (3.36) as an eigenvalue equation

$$\Sigma(\rho^{T_B})^* \Sigma \rho^{T_B} |\phi\rangle = \frac{\mu^2}{4} |\phi\rangle. \quad (3.37)$$

In Appendix B (Lemma 6), we show that the smallest eigenvalue γ of $Y = \Sigma(\rho^{T_B})^* \Sigma \rho^{T_B}$ is given by $\gamma = c^2(\rho)/4$, where $c(\rho)$ is the concurrence of ρ . Furthermore, it follows from Lemma 7 that $\mu^2/4$ is the smallest eigenvalue of Y , since $\langle \phi | \rho^{T_B} | \phi \rangle < 0$ according to Eq. (3.36). \square

C. Proof of the Corollary

Let ρ be an entangled state with $\text{rank}(\rho) < 4$, and $\rho = (1 - \lambda)|\psi\rangle\langle\psi| + \lambda\rho_s$ its optimal decomposition. Furthermore, we define $\rho_\epsilon := (1 - \epsilon)\rho + \epsilon\mathbb{I}/4$ (where \mathbb{I} is the 4×4 identity operator). Obviously, $\text{rank}(\rho_\epsilon) = 4$ and $\rho = \lim_{\epsilon \rightarrow 0} \rho_\epsilon$. Since the optimal decomposition of ρ_ϵ varies continuously with ϵ , it follows from Theorem 1 in the limit $\epsilon \rightarrow 0$ that

$$\exists_{|\phi\rangle} \rho_s^{T_B} |\phi\rangle = 0, \quad \exists_{|\tilde{\phi}\rangle} \rho_s |\tilde{\phi}\rangle = 0, \quad \text{and } \exists_{\alpha, \nu \geq 0} \left[\nu |\tilde{\phi}\rangle\langle\tilde{\phi}| + [|\phi\rangle\langle\phi|]^{T_B} \right] |\psi\rangle = -\alpha |\psi\rangle. \quad (3.38)$$

This equation includes both cases (i) and (ii) of Theorem 1. (In the former case, $\nu = 0$ and $|\tilde{\phi}\rangle$ is an element of the kernel of ρ_s .) On the other hand, if we assume that $|\phi\rangle$ is not a product vector (i.e. $c(\phi) > 0$), then Eq. (3.38) is sufficient for the optimality of the decomposition. This can be proven in the same way as above in the proof of the reverse direction of Theorem 1. Indeed, no assumption about the rank of ρ is needed there, except for showing that $|\phi\rangle$ is not a product vector (which ensures that $-\alpha$ is strictly the smallest eigenvalue of $A = \nu |\tilde{\phi}\rangle\langle\tilde{\phi}| + [|\phi\rangle\langle\phi|]^{T_B}$). It remains to be shown that $c(\phi) > 0$ is necessary for the optimality of the decomposition. For this purpose, let us assume that $|\phi\rangle = |e, f\rangle$ is a product vector. From the definition of partial transposition, we know that $\rho_s |e, f^*\rangle = 0$, and from Eq. (3.38) with $\alpha \geq 0$ that $|\psi\rangle \perp |e, f^*\rangle$. This implies $\rho |e, f^*\rangle = 0$. Then, it is easy to show that the BSA of $\rho_\delta := (1 - \delta)\rho + \delta |e, f^*\rangle\langle e, f^*|$ is given by $\rho_{\delta_s} = (1 - \delta)\rho_s + \delta |e, f^*\rangle\langle e, f^*|$. Hence, any vector $|\phi_\delta\rangle$ with $\rho_{\delta_s}^{T_B} |\phi_\delta\rangle = 0$ fulfills $|\phi_\delta\rangle \perp |e, f\rangle$, which, in the limit $\delta \rightarrow 0$, contradicts the assumption $|\phi\rangle = |e, f\rangle$. \square

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APPENDIX A

In the Appendix we formulate and prove several Lemmas used in the main part of the paper.

Lemma 1. Let ρ_s be a two qubit density matrix. If $\text{rank}(\rho_s^{T_B}) \leq 2$, then $\text{rank}(\rho_s) = \text{rank}(\rho_s^{T_B})$.

Proof: Since every two-dimensional subspace contains a product vector [1], also the kernel of $\rho_s^{T_B}$ must do so, i.e. $\rho_s^{T_B}|e, f\rangle = 0$. It follows that $\rho_s|e, f^*\rangle = 0$. Indeed, from (2.5) we have $\langle e, f^*|\rho|e, f^*\rangle = \langle e, f|\rho^{T_B}|e, f\rangle = 0$, and since ρ_s as a density matrix is positive definite, $\rho|e, f^*\rangle = 0$. By local unitary transformations in both subspaces we can choose $|e, f^*\rangle = |0, 0\rangle = |e, f\rangle$. Equations $\rho|0, 0\rangle = 0$ and $\rho^{T_B}|0, 0\rangle = 0$ together with hermiticity of both matrices leave only six nonvanishing elements in each of them, and by inspection one checks that their characteristic polynomials (hence also the spectra) are identical.

Lemma 2. For an arbitrary $|\phi\rangle$ the matrix $[|\phi\rangle\langle\phi|]^{T_B}$ has eigenvalues

$$-\frac{c}{2}, \frac{c}{2}, \frac{1 - \sqrt{1 - c^2}}{2}, \frac{1 + \sqrt{1 - c^2}}{2},$$

where $c = c(\phi)$ is the concurrence of $|\phi\rangle$. If $c > 0$, the eigenvector belonging to the negative eigenvalue is maximally entangled.

Proof: The first part of the Lemma is proven by an explicit calculation. In order to prove the second statement, let $L = U \otimes V$ be a local transformation, and $|\phi'\rangle = L|\phi\rangle$. Then

$$[|\phi'\rangle\langle\phi'|]^{T_B} = L'[|\phi\rangle\langle\phi|]^{T_B}L'^{\dagger},$$

where $L' = U \otimes V^*$. Observe that L' is a local transformation, hence it does not influence the concurrence of vectors. Now,

$$[|\phi\rangle\langle\phi|]^{T_B}|\psi\rangle = -\frac{c(\phi)}{2}|\psi\rangle \Leftrightarrow [|\phi'\rangle\langle\phi'|]^{T_B}|\psi'\rangle = -\frac{c(\phi)}{2}|\psi'\rangle, \quad (\text{A1})$$

where $|\psi'\rangle = L'|\psi\rangle$. Let us now choose L such that it brings $|\phi\rangle$ to its Schmidt basis:

$$|\phi'\rangle = L|\phi\rangle = \begin{bmatrix} \lambda_1 \\ 0 \\ 0 \\ \lambda_2 \end{bmatrix}.$$

It is now straightforward to show that $|\psi'\rangle$ in (A1) has the form

$$|\psi'\rangle = \frac{1}{\sqrt{2}}e^{i\delta} \begin{bmatrix} 0 \\ 1 \\ -1 \\ 0 \end{bmatrix}, \quad (\text{A2})$$

hence $|\psi'\rangle$ is maximally entangled and the same is true about $|\psi\rangle$ which is obtained from $|\psi'\rangle$ by a local transformation L' .

(Similar versions of Lemma 1 and Lemma 2 can also be found in [12].)

Lemma 3. If $|\psi\rangle$ is maximally entangled then

$$[|\psi\rangle\langle\psi|]^{T_B} = \frac{1}{2}\mathbb{I} - |\tilde{\psi}\rangle\langle\tilde{\psi}|, \quad (\text{A3})$$

where \mathbb{I} is the 4×4 identity operator and $|\tilde{\psi}\rangle$ is the eigenvector of $[|\psi\rangle\langle\psi|]^{T_B}$ with the negative eigenvalue i.e.

$$[|\psi\rangle\langle\psi|]^{T_B}|\tilde{\psi}\rangle = -\frac{1}{2}|\tilde{\psi}\rangle. \quad (\text{A4})$$

According to Lemma 2, $|\tilde{\psi}\rangle$ is maximally entangled.

Proof: Since $[|\psi\rangle\langle\psi|]^{T_B}$ is Hermitian, it has, in addition to $|\psi_4\rangle := |\tilde{\psi}\rangle$ three other orthogonal eigenvectors $|\psi_i\rangle$, $i = 1, 2, 3$ fulfilling, according to Lemma 2

$$[|\psi\rangle\langle\psi|]^{T_B}|\psi_i\rangle = \frac{1}{2}|\psi_i\rangle, \quad i = 1, 2, 3. \quad (\text{A5})$$

Using (A5) and (A4) together with the orthonormality of the eigenvectors, $\langle\psi_i|\psi_j\rangle = \delta_{ij}$, $i = 1, 2, 3, 4$, one sees that the actions of both sides of (A3) give the same results on the complete orthonormal set $|\psi_i\rangle$, $i = 1, 2, 3, 4$, which establishes the (A3) as a matrix equation.

Lemma 4. For arbitrary $|\phi\rangle$,

$$\max_{m.e.} |\langle\phi|\psi\rangle|^2 = \frac{1}{2} + \frac{1}{2}c(\phi), \quad (\text{A6})$$

where the maximum is taken over all maximally entangled $|\psi\rangle$. The maximum is attained if $|\psi\rangle$ and $|\phi\rangle$ have a common Schmidt basis.

Proof: By a local unitary transformation (which does not change neither $|\langle\phi|\psi\rangle|^2$ nor the entanglements of $|\phi\rangle$ and $|\psi\rangle$) we can bring $|\phi\rangle$ to its Schmidt basis:

$$|\phi\rangle = \begin{bmatrix} \lambda_1 \\ 0 \\ 0 \\ \lambda_2 \end{bmatrix}, \quad \lambda_i \geq 0, \quad \lambda_1^2 + \lambda_2^2 = 1.$$

Using the general form (2.9) of a maximally entangled state, we conclude that in the new basis

$$|\langle\phi|\psi\rangle|^2 = |a_1\lambda_1 \pm a_1\lambda_2|^2 \leq |a_1|^2 (\lambda_1 + \lambda_2)^2 = |a_1|^2 (1 + 2\lambda_1\lambda_2) = |a_1|^2 [1 + c(\phi)],$$

and the maximum is attained if $|a_1|^2$ is maximal, i.e. $|a_1|^2 = 1/2$ and $a_2 = 0$, which completes the proof.

Lemma 5. Let $|\phi\rangle$ be an entangled state and $|\psi\rangle$ the eigenvector of $[|\phi\rangle\langle\phi|]^{T_B}$ with the negative eigenvalue i.e.

$$[|\phi\rangle\langle\phi|]^{T_B}|\psi\rangle = -\frac{c(\phi)}{2}|\psi\rangle, \quad (\text{A7})$$

Then $|\phi\rangle$ and $|\tilde{\psi}\rangle$ have a common Schmidt basis, where $|\tilde{\psi}\rangle$ is the eigenvector of $[|\psi\rangle\langle\psi|]^{T_B}$ with the negative eigenvalue, i.e.

$$[|\psi\rangle\langle\psi|]^{T_B}|\tilde{\psi}\rangle = -\frac{1}{2}|\tilde{\psi}\rangle.$$

Proof: From (A7) we have

$$-\frac{c(\phi)}{2} = \langle\psi| [|\phi\rangle\langle\phi|]^{T_B} |\psi\rangle = \text{Tr}([|\phi\rangle\langle\phi|]^{T_B} |\psi\rangle\langle\psi|) = \text{Tr}(|\phi\rangle\langle\phi| [|\psi\rangle\langle\psi|]^{T_B}) = \langle\phi| [|\psi\rangle\langle\psi|]^{T_B} |\phi\rangle.$$

From Lemma 2 we know that $|\psi\rangle$ is maximally entangled. Thus, according to Lemma 3, in the last term we can substitute $[|\psi\rangle\langle\psi|]^{T_B}$ by $\frac{1}{2}\mathbb{I} - |\tilde{\psi}\rangle\langle\tilde{\psi}|$, consequently:

$$\langle\phi|\tilde{\psi}\rangle\langle\tilde{\psi}|\phi\rangle = \frac{1}{2} + \frac{c(\phi)}{2},$$

hence, from Lemma 4, $|\phi\rangle$ and the maximally entangled $|\tilde{\psi}\rangle$ have a common Schmidt basis.

APPENDIX B

Lemma 6. If ρ is an entangled state, i.e. its concurrence $c(\rho)$ is positive, then $c^2(\rho)/4$ equals the smallest eigenvalue of $Y = \Sigma(\rho^{T_B})^* \Sigma \rho^{T_B}$.

Proof: If $d_1^2/4, \dots, d_4^2/4$ are the eigenvalues of $Y = \Sigma(\rho^{T_B})^* \Sigma \rho^{T_B}$ and $c_1^2 \geq \dots \geq c_4^2$ the (real and positive, see [3]) eigenvalues of $X = \Sigma \rho^* \Sigma \rho$ (c.f. Eq. (2.7)), the following relation holds:

$$\begin{aligned}
d_1^2 &= (c_1 + c_2 + c_3 - c_4)^2, \\
d_2^2 &= (c_1 + c_2 - c_3 + c_4)^2, \\
d_3^2 &= (c_1 - c_2 + c_3 + c_4)^2, \\
d_4^2 &= (-c_1 + c_2 + c_3 + c_4)^2.
\end{aligned}$$

Indeed, invoking the anticommutation relations for Pauli matrices, we check that for an arbitrary local transformation $L = U \otimes V$, $U, V \in SU(2)$

$$L^* = \Sigma L \Sigma. \quad (\text{B1})$$

We can thus use local transformations to bring ρ in $X = \Sigma \rho^* \Sigma \rho$ and $Y = \Sigma(\rho^{T_B})^* \Sigma \rho^{T_B}$ to a relatively simple form. An arbitrary hermitian ρ can be decomposed as

$$\rho := \frac{1}{4} \mathbb{I}_4 + \sum_k (a'_k \sigma_k \otimes \mathbb{I}_2 + b'_k \mathbb{I}_2 \otimes \sigma_k) + \sum_{nm} C_{nm} \sigma_m \otimes \sigma_n, \quad (\text{B2})$$

with real a'_k, b'_k , and C_{mn} . By local transformations, we can bring the 3×3 matrix C to the diagonal form with nonnegative diagonal elements μ_1, μ_2 , and μ_3 [13,14]. The desired transformation changes a'_k and b'_k to some other real a_k and b_k , hence finally

$$\rho = \frac{1}{4} + \begin{bmatrix} a_3 + b_3 + \mu_3 & b_1 - ib_2 & a_1 - ia_2 & \mu_1 - \mu_2 \\ b_1 + ib_2 & a_3 - b_3 - \mu_3 & \mu_1 + \mu_2 & a_1 - ia_2 \\ a_1 + ia_2 & \mu_1 + \mu_2 & -a_3 + b_3 - \mu_3 & b_1 - ib_2 \\ \mu_1 - \mu_2 & a_1 + ia_2 & b_1 + ib_2 & -a_3 - b_3 + \mu_3 \end{bmatrix}. \quad (\text{B3})$$

Somewhat tedious but straightforward calculations show that

$$\text{Tr} Y = \text{Tr} X \quad (\text{B4})$$

$$\text{Tr} Y^2 = \text{Tr} X^2 - \delta_2 \quad (\text{B5})$$

$$\text{Tr} Y^3 = \text{Tr} X^3 - \delta_3 \quad (\text{B6})$$

$$\text{Tr} Y^4 = \text{Tr} X^4 - \delta_4 \quad (\text{B7})$$

where

$$\delta_2 = 6d + \frac{3}{2} \text{Tr} X^2 - \frac{3}{4} (\text{Tr} X)^2, \quad (\text{B8})$$

$$\delta_3 = \frac{5}{4} \delta_2 \text{Tr} X, \quad (\text{B9})$$

$$\delta_4 = \frac{7}{12} \delta_2 (2 \text{Tr} X^2 + (\text{Tr} X)^2 - \delta_2), \quad (\text{B10})$$

$$d^2 = \det X. \quad (\text{B11})$$

On the other hand, as (this time rather short) calculations show, the same relations hold for two diagonal matrices

$$X' = \text{diag}(c_1^2, c_2^2, c_3^2, c_4^2), \quad Y' = \text{diag}(d_1^2, d_2^2, d_3^2, d_4^2)/4 \quad (\text{B12})$$

where

$$d_1^2 = (c_1 + c_2 + c_3 - c_4)^2, \quad (\text{B13})$$

$$d_2^2 = (c_1 + c_2 - c_3 + c_4)^2, \quad (\text{B14})$$

$$d_3^2 = (c_1 - c_2 + c_3 + c_4)^2, \quad (\text{B15})$$

$$d_4^2 = (-c_1 + c_2 + c_3 + c_4)^2, \quad (\text{B16})$$

if we choose $d = +(\det X)^{1/2}$, or

$$d_1^2 = (-c_1 + c_2 + c_3 - c_4)^2, \quad (\text{B17})$$

$$d_2^2 = (-c_1 + c_2 - c_3 + c_4)^2, \quad (\text{B18})$$

$$d_3^2 = (-c_1 - c_2 + c_3 + c_4)^2, \quad (\text{B19})$$

$$d_4^2 = (c_1 + c_2 + c_3 + c_4)^2, \quad (\text{B20})$$

if $d = -(\det X)^{1/2}$. Since there is a one to one correspondence between the set of eigenvalues of a n -dimensional matrix and the traces of its first n powers, the relation between the eigenvalues c_i^2 of X and the eigenvalues $d_i^2/4$ of Y must be given by (B13–B16) or (B17–B20). The second case, $d < 0$, is excluded due to the positivity of ρ . Indeed, one checks that:

$$d = \frac{1}{6}\delta_2 - \frac{1}{4}\text{Tr}X^2 + \frac{1}{8}(\text{Tr}X)^2 = \det(\rho) \geq 0. \quad (\text{B21})$$

The first equality in (B21) follows from (B8) whereas the second is established by an explicit calculation using (B3) and the definition of X in terms of ρ .

Thus the eigenvalues d_1^2, \dots, d_4^2 (B13–B16) of $4Y$ are real and positive, and the smallest eigenvalue d_4^2 equals $c(\rho)^2$, see Eq. (2.6).

Lemma 7. If $\text{rank}(\rho) \geq 3$, where ρ is an entangled state, the smallest eigenvalue of $Y = \Sigma(\rho^{T_B})^* \Sigma \rho^{T_B}$ is non-degenerate. If $|\phi_4\rangle$ denotes the corresponding eigenvector, and $|\phi_i\rangle$, $i = 1, 2, 3$, the other three eigenvectors, the following holds:

$$\langle \phi_4 | \rho^{T_B} | \phi_4 \rangle = -\frac{1}{2}c(\rho)c(\phi_4), \quad (\text{B22})$$

$$\langle \phi_i | \rho^{T_B} | \phi_i \rangle \geq 0, \quad i = 1, 2, 3. \quad (\text{B23})$$

Proof: Let $d_1^2/4 \geq \dots \geq d_4^2/4$ denote the (real and positive, see Lemma 6) eigenvalues of Y , and $c_1^2 \geq \dots \geq c_4^2$ the eigenvalues of $X = \Sigma \rho^* \Sigma \rho$. According to Lemma 6, the relation between d_i and c_i is given by Eqs. (B13–B16), in particular $d_4 = c(\rho)$. From $c(\rho) > 0$ and the definition of concurrence, Eq. (2.6), it follows that $c_1 > c_2$. Now, if $\text{rank}(\rho) \geq 3$, it is easy to show that $c_2 > 0$ (since $\text{rank}(\Sigma) = 4$ and therefore $\text{rank}(X) \geq 2$), and then Eqs. (B15, B16) imply $d_4 < d_3$. Hence, $d_4^2/4$ is a non-degenerate eigenvalue.

By splitting the eigenvalue equation $Y|\phi_i\rangle = \frac{1}{4}d_i^2|\phi_i\rangle$ (with real d_i) into its real and imaginary part, one can derive that $|\phi_i\rangle$ fulfills $\Sigma \rho^{T_B} |\phi_i\rangle = \frac{1}{2}e^{i\chi_i} d_i |\phi_i^*\rangle$, where $e^{i\chi_i}$ is a phase factor. Using $\Sigma^2 = 1$, Eq. (2.8), and the hermiticity of ρ^{T_B} , we conclude that

$$\langle \phi_i | \rho^{T_B} | \phi_i \rangle = \pm \frac{1}{2} d_i c(\phi_i). \quad (\text{B24})$$

In order to complete the proof of Lemma 7, it remains to be shown that the sign on the right hand side must be negative for $i = 4$ and nonnegative for $i = 1, 2, 3$. Because of continuity, it is sufficient to consider the case $\text{rank}(\rho) = 4$. Then, $|\phi_i\rangle$ cannot be a product vector (since inserting $|\phi_i\rangle = |e, f\rangle$ into Eq. (B24) would imply $\langle e, f^* | \rho | e, f^* \rangle = 0$), i.e. the right hand side of Eq. (B24) cannot be zero ($d_i > 0$ follows from $d_4 = c(\rho) > 0$). Now, if ρ is infinitesimally close to an entangled pure state, $\rho \rightarrow |\psi\rangle\langle\psi|$, it is easy to check that, indeed, Eq. (B24) is valid with the minus sign for $i = 4$ and the plus sign for $i = 1, 2, 3$. (For $|\psi\rangle = [\lambda_1, 0, 0, \lambda_2]^T$, one finds that $|\phi_{1,2}\rangle = [\lambda_2, 0, 0, \pm\lambda_1]^T$, $|\phi_3\rangle = [0, 1, 1, 0]^T/\sqrt{2}$, and $|\phi_4\rangle = [0, 1, -1, 0]^T/\sqrt{2}$.) Next, we consider the one parameter family $\rho(\lambda') = \mu'|\psi\rangle\langle\psi| + \lambda'\rho_s$, with $\mu' = 1 - \lambda'$ and $\lambda' \in [0, \lambda]$, where ρ_s is the BSA of $\rho = \rho(\lambda)$. Since $\rho_s^{T_B}$ is positive, $\langle \chi | \rho^{T_B} | \chi \rangle < 0$ implies $\langle \chi | \rho(\lambda')^{T_B} | \chi \rangle < 0$, hence $c(\rho(\lambda')) > 0$ for all $\lambda' \in [0, \lambda]$. Finally, continuity implies that the sign of the right hand side of Eq. (B24) does not change when increasing λ' from 0 to λ .

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